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CITATION:

Tokimatsu, Koji ...[et al]. Energy modeling approach to the global energy-mineral nexus: Exploring metal requirements and the well-below 2°C target with 100 percent renewable energy. Applied Energy 2018, 225: 1158-1175

ISSUE DATE:

2018-09-01

URL:

http://hdl.handle.net/2433/234595

Applied Energy 225 (2018) 1158–1175

Contents lists available at ScienceDirect

Applied Energy

journal homepage: www.elsevier.com/locate/apenergy

Energy modeling approach to the global energy-mineral nexus: Exploring metal requirements and the well-below 2 °C target with 100 percent renewable energy

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HIGHLIGHTS

- Original "100% Renewable" scenario was added to "Coal & Nuclear, Gas & Renewable".
- Fully decarbonization in all sectors was essential to meet the well-below 2 °C target.
- Metal requirement was estimated with several uncertainties across the scenarios.
- Vanadium was identified as *distinctly* critical metal.

ARTICLE INFO

Keywords:
2 °C target
100% Renewable energy scenario
Energy-mineral nexus
Zero emissions
Metal requirement
Hydrogen

ABSTRACT

Detailed analysis of pathways to future sustainable energy systems is important in order to identify and overcome potential constraints and negative impacts and to increase the utility and speed of this transition. A key aspect of a shift to renewable energy technologies is their relatively higher metal intensities. In this study a bottom-up cost-minimizing energy model is used to calculate aggregate metal requirements in different energy technology including hydrogen and climate policy scenarios and under a range of assumptions reflecting uncertainty in future metal intensities, recycling rate and life time of energy technologies. Metal requirements are then compared to current production rates and resource estimates to identify potentially "critical" metals. Three technology pathways are investigated: 100 percent renewables, coal & nuclear and gas & renewables, each under the two different climate policies: net zero emissions satisfying the well-below 2 °C target and business as usual without carbon constraints, resulting together in six scenarios. The results suggest that the three different technology pathways lead to an almost identical degree of warming without any climate policy, while emissions peaks within a few decades with a 2 °C policy. The amount of metals required varies significantly in the different scenarios and under the various uncertainty assumptions. However, some can be deemed "critical" in all outcomes, including Vanadium. The originality of this study lies in the specific findings, and in the employment of an energy model for the energy-mineral nexus study, to provide better understanding for decision making and policy development.

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https://doi.org/10.1016/j.apenergy.2018.05.047
Received 31 December 2017; Received in revised form 24 April 2018; Accepted 10 May 2018
Available online 01 June 2018

1. Introduction

1.1. Background

Renewable energy and the hydrogen economy have long been expected to substitute for non-renewable energy resources, for various reasons such as meeting sustained energy demand or climate policy targets. However, little consideration has been given to the many mineral resources used in the energy technologies required to meet future energy needs and climate policy. To the authors' knowledge, few modeling exercises have been undertaken using bottom-up technology type assessments to address the energy-mineral nexus, specifically examining potentially scarce metals in technologies for renewable and hydrogen energy. In our previous study [1], we stressed the importance of the nexus approach using bottom-up energy modeling because of its flexibility in energy scenario development and its ability to estimate metal requirements, however, further assessment to meet the well-below 2 °C or 1.5 °C targets, especially "radical" or "extreme" scenarios such as 100% renewable energy scenarios were not addressed. Such stringent climate policy further endorses the need for expanding variable renewable energy in power systems combined with energy storage, and promoting competitiveness in automobile energy storage, batteries (electric vehicles; EV) and hydrogen tanks (fuel cell vehicles; FCV). Bottom-up global energy models are compatible for illustrating coarse (or rough) sketches with such global trends in energy and climate policies taken into consideration.

1.2. Research objectives and originalities

In this study we address (i) meeting the well-below 2 °C target including non-carbon greenhouse gases (NCGHGs) (ii) by creating a new 100% renewable energy (denoted as Ren 100) scenario in addition to our previous two energy scenarios (i.e., Coal & Nuc, Gas & Ren) [1] (iii) to clarify the metal requirements including hydrogen related technologies while our past study only focus on those for power generation. All of these are considered to be points of originality, as well as the employment of our energy model for the energy-mineral nexus study. To our knowledge, detailed 100% renewable energy scenarios have not been adequately addressed at the global level [2,3], although there have been many such studies at local or national levels [4–9].

The structure of this article is as follows. Section 2 provides a literature review for hydrogen energy, as it is a potential technology that has widely been incorporated in global detailed studies [10] without addressing their metal requirement. Section 3 describes our model and assumptions for metal requirements and availability. Sections 4 and 5 present the results and discussion, respectively. Section 6 concludes this study.

2. Literature review of industrial hydrogen

Hydrogen is unavailable in pure form from any natural deposits. It has to be synthesised to purity levels that match demand specifications from various technological applications (Table 1). Hydrogen can be generated in both gaseous and liquid forms at production sites and the desired purity level has a significant impact on the production cost. Hydrogen has been seen as a useful potential energy carrier for some time, in particular, since the modern inception of the Hydrogen Economy concept in the 1960s and early 1970s, which foresaw the use of renewable energy to produce hydrogen mainly for use in transportation for the strengthening of energy security [11]. Hydrogen is seen as having the advantage of being obtainable from water using any form primary energy [12].

On the demand side, hydrogen is usable in fuel cells of various types, internal combustion engines and gas turbines, as well as other combustion processes or as a chemical feedstock. Between supply and demand, one must also consider the various storage and transportation methods – liquid storage, compressed gas, metal hydride, aromatic and other multi-bond organics, carbon nanotubes and activated carbon. The main processing routes – from primary energy source through to utilization – are shown in Fig. 1. It is worth pointing out that ammonia production accounts for roughly 50% of all hydrogen consumption and together with petroleum processing, and methanol synthesis about 90% of world hydrogen consumption is accounted for [13–15].

Table 1
Hydrogen purity level classification and typical uses.
Adapted from CertifHy [15].

Gaseous (Type I)		Liquid (Type II)	
Typical uses	Hydrogen purity [%]	Typical uses	Hydrogen purity [%]
General industry applications	99.95	Industrial, fuel and standard propellant	99.995
Hydrogenation and water chemistry	99.99	High purity, industrial, fuel and propellant	99.999
Instrumentation and propellant	99.995	Semiconductor uses	99.9997
Semiconductor, specialty uses	99.999		

2.1. Current and future hydrogen supply

Currently, global production is about 65 million metric tons of H2 generated from different sites using various production technologies. However, roughly 98% of all hydrogen production relies on fossil fuels directly as feedstock (i.e. reforming, partial oxidation, etc.) or indirectly via electricity and process heat that are chiefly derived from fossil fuels [16]. Hydrogen can be technically produced from various feedstocks by gasification, pyrolysis or reforming as well as by electrolysis of water or via a variety of microbial photocatalytic processes as presented more fully in Appendix A. For more comprehensive reviews one may read Kothari et al. [17], Muradov and Veziruglo [18], and Muradov [16].

Industrial hydrogen production will remain heavily dependent – both directly and indirectly – on fossil fuels for the foreseeable future. It is possible to use non-fossil electricity and heat for the process in some cases, but many reforming technologies rely on methane, light hydrocarbons or off-gas streams from fossil fuel processing that is hard to replace without fundamental restructuring of significant proportions of the existing hydrogen industry. Electricity-driven processes such as plasma reforming or water electrolysis could be promising, but have significantly higher CO_2 emissions unless larger parts of the global electricity mix simultaneously become decarbonized [16].

2.2. Critical materials for the hydrogen economy

Available literature provides an ample number of minerals that are being examined for potential use in the hydrogen economy. However, of those materials that are relatively widely used at present in hydrogen technologies, there are a number that are considered critical by various countries. Broadly speaking, nickel, lithium, platinum group metals (PGMs) and rare earth elements including yttrium (REEs) are perhaps the most important among these, covering various technologies of the hydrogen supply chain and being somewhat difficult to substitute. The known reserves and resources of these minerals are in general considered sufficient for current demand [19,20], but the potential for significant demand shift due to hydrogen economy expansion should be examined.

Critical materials required for specific hydrogen supply chain technologies were identified from a broad literature review of experimental, commercial and lifecycle assessment (LCA) articles reporting the materials used and corresponding performance of various

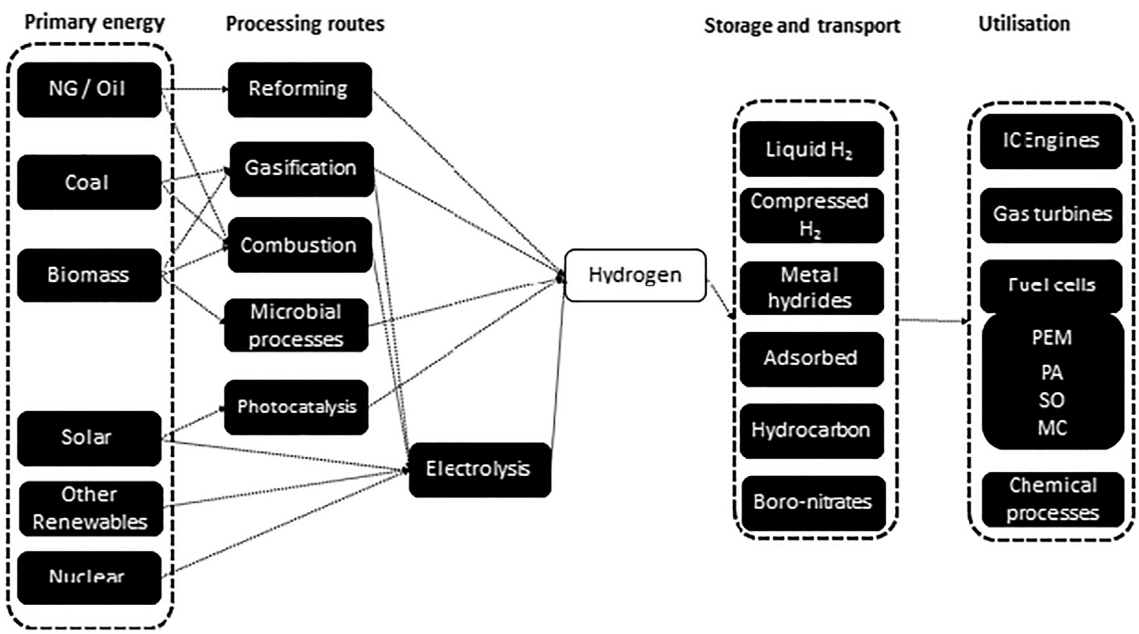

Fig. 1. Main hydrogen supply chain configurations.

technologies. Because of the large body of literature examined and the limitations of space, only representative articles are cited. Of the many minerals that can potentially be used in a hydrogen economy, in this case we highlight those minerals that are considered critical by more than one of Japan, Korea, UK and USA (as compiled elsewhere [21]). Bulk minerals – whilst key to all energy infrastructure – are ignored for the time being.

There is unavoidable error in utilizing this type of data – experimental data may be overly optimistic of performance or overly pessimistic of materials intensity due to its early stage of development; commercial data is often insufficiently detailed and can be overly optimistic; LCA data is sometimes underspecified and can also tend to be out-of-date, and in some cases may be country-specific. In any case, there is a necessity to critically analyse the data available, utilizing the sources and values considered to be most appropriate. In this case, quantification is not yet presented, as a more thorough database examination is required. However, the qualitative aspects of specific mineral resource constraints are discussed.

2.2.1. Key materials for hydrogen supply

There are a variety of key minerals that are used for catalysts and membranes for hydrogen production and purification. Photocatalysis has largely focused around common materials such as TiO_2 and alloys, but some rarer elements such as gallium have also been utilized. Gallium is a relatively small-production by-product metal, and would potentially pose a risk to supply if required either directly in photocatalysts, or in thin-film solar cells to power conventional electrolysis ([22,23]).

Catalysts utilized in steam reforming of natural gas, and in the water gas shift reaction are traditionally based on the metals nickel, rhodium, platinum, and different Rh/Pt-alloys of on various supports [24]. In recent decades, noble metal catalysts have been extensively explored due to their affinity for high conversion efficiencies and high H_2 selectivity. However, recent trends indicate that research focus has now shifted to the development of non-noble metal catalysts and this is primarily driven by the associated costs that adversely impact market acceptability when using noble metals [25].

Nickel is often the most frequently used, but can have challenges with activity and with vulnerability to sulphur [26]. This can be somewhat overcome by combination with compounds such as Ce, Zr, but even different PGMs (primary Ru/Pt/Pd/Rh) suffer significant and often irreversible degradation in sulphur atmospheres. Also within off-gas hydrogen, Ni is commonly used. One such example is the Ni-cathodes used by the chlor-alkali industry. Nickel is considered a critical mineral from the perspective of Korea and Japan, but more importantly, the substitute materials and doping elements may be even more critical.

Membrane reactors and membranes for the separation or purification of hydrogen have been widely proposed, with most utilizing Pd as a membrane material. This material has a variety of constraints – foremost is its relatively high cost, but it is also vulnerable to degradation through reaction with sulphur. It has been successfully alloyed with copper, cerium, indium, ruthenium and silver among others [27]. Vanadium, tantalum and niobium have also been combined with Pd for hydrogen separation. Electrolysis cells are often effectively fuel cells run in reverse, and hence the mineral requirements tend to mimic those of fuel cells, as discussed below.

Metal hydrides for hydrogen storage are often based on lithium alloys to reduce weight constraints [28]. More importantly perhaps, are the alloying requirements for pipelines to transport hydrogen – generally nickel-based alloys or austenitic steels that are likely to be more costly and could potentially put more strain on nickel reserves.

2.2.2. Critical materials for fuel cells

Each type of fuel cell has its own limitations, as well as a variety of key mineral components. One of the most widely recognized issues with Polymer Electrolyte Membrane Fuel Cells (PEMFC), is the platinum content in the electrodes [29]. The amounts required have been largely reduced over time through research efforts, and further progress could be expected.

Molten Carbonate fuel cells (MCFC) often contain lithium, as well as utilizing Ni and Cr in the electrodes [30]. Lithium is considered to be a critical metal by many countries, for many current and emerging uses – particularly in batteries in recent years. While there are still very significant reserves and resources available, the production capacity is currently lagging, and the potential of future production dependence on Latin America has been raised as a potential risk [31,32].

Solid Oxide Fuel Cells (SOFC) often use Lanthanum and Yttria-stabilised Zirconia (YSZ) as component materials. Yttria is often considered with the rare earth elements (REE), and therefore may be of some concern [33]. Zirconium is not seen as a critical mineral by most countries, but is vitally important as a cladding material in nuclear reactors, among other uses. Strontium is also often utilized, but again is not widely considered to be critical. Previous examination of rapid expansion of the use of PEMFC or

SOFC with constraints on reserves of PGM and REE indicated some lag, but little real restriction, on the supply of minerals for fuel cells [34].

3. Methodology

3.1. Applied model

3.1.1. Outline of the overall model

The global model applied here consists of three hard-linked models (Fig. 2) composed of a simplified climate model with the following resources: energy (or fuel minerals, fossil and uranium), minerals (non-fuel minerals used for materials production), and biomass and food. Unlike for example the *World model* using a system dynamic techniques in the *Limits to Growth* study [35], our model applying linear programing is a type of bottom-up technology model comparable to the MARKAL/TIMES/TIAM families[1] [38]. However, a distinct feature of the model applied here is the inclusion of the mineral resource balance model that is not typically incorporated. One of the strengths of this design is the ability to discuss for example the copper requirement compared with its demand endogenously obtained from the mineral model. A weakness on the other hand is the exclusion of detailed end-use technologies (e.g., lighting) that are covered in the MARKAL family [39].

The model provides a consistent structure for supplying the resources to meet exogenous demand scenarios.[2] The upper section of Fig. 2 illustrates the mineral and material flows, the lower section shows biomass and food flows, and the middle section shows energy flows. These three sections correspond to the three resource models for the balance of materials, biomass and food via land use, and energy systems, respectively. The right side shows demand together with end-use products and waste disposal while the left side indicates resource supply.

The black lines show material flows, with solid lines representing mainstream industry, both dot-dashed and dashed lines represent biomass residues and scrap materials, and peripheral or recycling industry, respectively. The blue, red, green, and orange lines indicate flows to meet the demands for electricity, heat, and transportation via hydrogen and liquid fuels, respectively, while the dotted and solid lines indicate flows of energy resources and their products, respectively.

3.1.2. Objective function

The modeling approach used here is predicated on perfect foresight, assuming that costs and expansion rates of technologies[3] are known and can be taken into account via linear programing optimization. This idealized approach provides consistent, economically efficient future scenarios of technology deployment and resource allocation to meet climate or other policy targets.

Our global model framework consists from 10 regional areas or groups[4] (*rg*) with time horizons between 2010 and 2150 at 10-year intervals[5] (*yr*). The objective function of the overall model is formulated as the discounted sum, by using a discount rate (ρ) of 2% per annum and a 10-year time step (ξ), consisting of the total supply costs (*TC*) of energy resources (cost of fuel; fossil plus uranium: *FC*), non-fuel minerals and materials (non-fuel mineral and materials cost: *NFC*), and biomass and food (land cost: *LC*) :

$$TC = \sum_{\xi=0}^{14}\left(\frac{1}{1+\rho}\right)^{10\xi}\cdot\sum_{rg}(FC_{rg,2010+10\cdot\xi} + NFC_{rg,2010+10\cdot\xi} + LC_{rg,2010+10\cdot\xi}). \tag{1}$$

where details of *FC*, *NFC*, and *LC* are described in our publications elsewhere [1,40–42]. The linear programming consists of three sets of equations: an objective function, constraint equations, and balance equations. The objective function (*C*) is generally formulated by the sum of the products of decision variables (x_j) determined via optimization (minimization of cost) and the cost coefficients (c_j):

$$\min C = \sum_j c_j \times x_j. \tag{2}$$

Some description of cost data, constraints, and parameter settings is given here. Cost data are gathered from numerous publications (e.g., series of the IPCC special reports, the projected cost of generating electricity) for energy conversion technologies (including performance data), land cost, and fuel and mineral resources. In the energy modeling and mineral resource balance modeling, energy flows and material flows/stocks are determined by a least-cost algorithm on technology choice and resource production, whereas the land-use model flow of biomass and food resources is distributed by parameter settings, the decision variable of land area, such as crop land, is determined by the algorithm. Regarding examples of constraints, power generation technologies were allocated to base, middle, and peak demand, within which common constraints on share of generation types were provided in all the six scenarios in this study. Finally on parameter settings, we also assumed a year of introduction and increase in conversion efficiency corresponding to anticipated technological improvements. Unlike energy, biomass and food, mineral resources do not disappear after the end of use of products. All the end-of-life products are assumed to be ideally collected (implying no illegal dumping). In the land use model the parameter settings including recovery rate are given for all the flows and their intersections, while in the mineral resource balance model determination of all parts of their balances and intersections including final disposal and recovery to use as old scrap are determined by the least-cost algorithm.

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[1] The MARKAL family of models have a long history, a world-wide community of users, and incorporate various functionalities and expansions such as flexible inputs and outputs, stochastic programming, and endogenous technology learning. See details publications from the IEA-ETSAP website (e.g., [36,37]).

[2] Energy electricity, heat, and transportation), materials electricity, machinery, transportation, construction, and civic infrastructure), food pork and chicken, lamb and beef, and cereals), and wood lumber and boards, paper, and fuel). Those demands except materials are functions expressed by demand versus income on a per capita basis using income elasticities, while for those in materials see [40] a decomposition approach was applied based on intensity of metal use and final product demand expressed by GDP and/or population.

[3] Technology options included following productions of power, liquids, hydrogen, heat, transportation, steel, non-ferrous metal, and cement. 28 types of power (8 types of fossil fuel (coal, integrated gasification combined cycle (IGCC), oil, and gas, without and with CO_2 capture), 4 types of biomass (co-firing and integrated gasification (IBGCC), without and with CO_2 capture), hydrogen, 5 types of nuclear energy (light water reactor (LWR), fast breeder reactor (FBR), three types of nuclear fusion), and 10 types of renewables (PV, CSP, SPSS, onshore wind, offshore wind, conventional hydropower and pump, small- and medium-scale hydropower, geothermal power, ocean wave and tidal power, and ocean thermal energy conversion (OTEC)); 15 types of liquids, including refined oil, ethanol (bioethanol by biomass residue fermentation, without and with CO_2 capture), methanol (coal, gas, and biomass residue), biodiesel, and FT synfuel (biomass liquefaction, coal, natural gas, and heat utilization of nuclear fusion for biomass residue, without and with CO_2 capture); 12 types of hydrogen production, including fossil (coal, oil, and gas, without and with CO_2 capture), biomass (gasification, without and with CO_2 capture), nuclear (high-temperature gas cooling reactor (HTGR) and heat utilization of nuclear fusion for biomass residue, without and with CO_2 capture), and renewable (electrolysis by large deployment of PV); 8 types of heat, including biomass (biomass pellet heating,

(*footnote continued*)
biomass heating with CHP (combined heat and power), biomass anaerobic digestion with CHP, and municipal solid waste with CHP), geothermal (conventional deep geothermal with CHP, advanced deep geothermal with CHP, and shallow geothermal heating and cooling), and solar; 11 types of transportation, including passenger car (internal combustion engine (ICE), plug-in hybrid electric vehicle (PHEV), electric vehicle (EV), and fuel cell vehicles (FCV)), bus (ICE and FCV), truck (ICE and FCV), aviation, marine, and rail; 8 types of steel production, including blast furnace with converter and electric furnace with directly reduced iron (DRI) for construction steel and mechanical machinery steel, with and without CO_2 capture; 5 types of non-ferrous metal production, including aluminum, copper (dry and leached), lead, and zinc; 4 types of cement kilns, including wet, dry, advanced dry, and advanced dry with CO_2 capture; and 3 types of cement mills, including Portland cement, blast furnace cement, and Portland fly-ash cement.

[4] North America, Western Europe, Japan, Oceania, China, Southeast Asia (including member countries of the Association of Southeast Asian Nations (ASEAN) and India), the Middle East and North Africa, Sub-Saharan Africa, Latin America, and the former Soviet Union and Eastern Europe.

[5] Specifically, 10-year intervals (*yr*) are 2010, 2020, …, 2150.

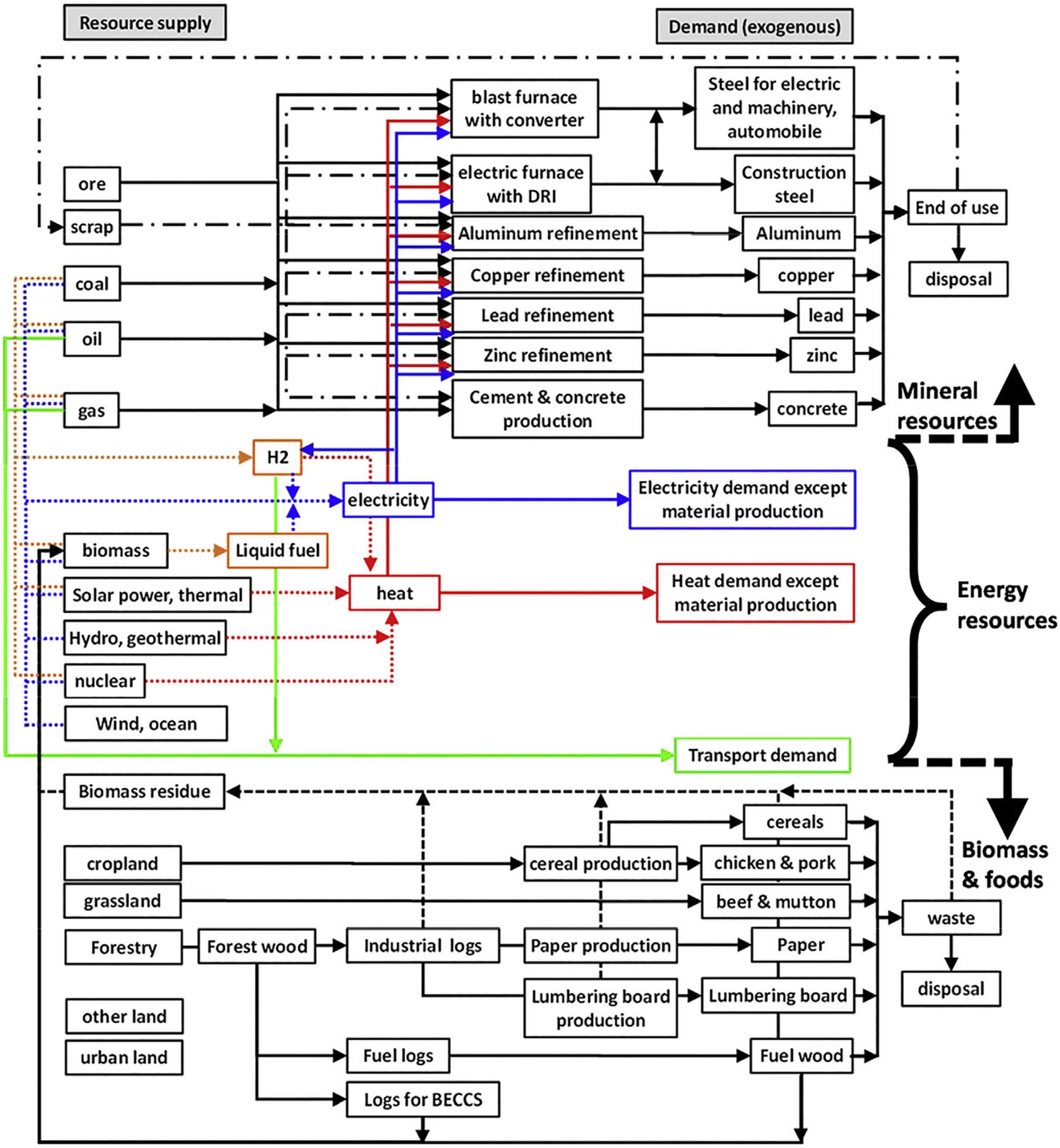

Fig. 2. The overall model structure.

3.2. The three energy pathways and two climate policies

Table 2a summarizes the three energy pathways that are modelled in this study to attain the well below 2 °C target including NCGHGs (below 1.8 °C). Unlike our previous study, all the sectors must be given the following constraints for decarbonization across the three energy pathways: all fossil-based technologies in the power and heat sectors must be equipped with carbon capture and storage (CCS) and hydrogen in aviation reaches 100% in 2100 via 50% in 2050. Table 2b presents changes in global mean temperature rise (GMTR) when relaxing the various constraints described below in the 100% renewable scenario.

Ren 100 is developed from an energy scenario dominated by gas and renewables (Gas & Ren) from our previous study [1]. The Ren 100 scenario cannot be built from Gas & Ren before allowing for the following additional settings and assumptions: (i) radical expansion in the allowable maximum share of renewables in the power sector, (ii) phasing out of nuclear and fossil fuel in production of hydrogen and liquid fuel in addition to the power and heating sectors by 2100.

The allowable maximum share of renewables in the power sector in Ren 100 is expanded compared with Gas & Ren as follows: 40% for each of photovoltaics (PV) and wind power (WP), this is more than doubled from 20% which also included ocean energy (i.e., PV, WP, ocean) in the Gas & Ren scenario. The allowable maximum share by ocean and biomass energy in Ren 100 is expanded by the amount of PV, WP, and oil from that of Gas & Ren (this can be understood by assuming 0% for PV, WP, and oil in Gas & Ren scenario in the Table 2a, arriving at a sum of percentages by ocean and oil equal to 30%). The Ren 100 scenario was considered to be inherently incompatible with nuclear power, hence nuclear phase-out is added. Phasing out of fossil fuels in the four sectors (power, heat, production of hydrogen and synfuel) are essential for the Ren 100 scenario. All the other settings including the maximum share by gas and coal (40% and 30% each) are common among the three

Table 2a
The three energy scenarios. (a) The Ren100 requires radical expansion in renewables and nuclear phase-out policy; changes are highlighted by grey.

Settings and assumption \ Energy scenarios	100% Renewable (Ren 100)	Gas & Renewables (Gas & Ren)	Coal & Nuclear (Coal & Nuc)
Fuel resources	Cheap Gas		Cheap Uranium
Power sector			
Nuclear phase-out policy	yes	no	
Renewables and fossil fired	numbers in below are maximum allowed share by each sector		
Renewables	40% by PV, WP	20% by PV, WP, ocean	
(PV, WP, ocean, bio)	30% by bio, ocean	10% by bio, oil	
Oil fired	10%		
Gas fired	40%		
Coal fired	30%		
deployment of CCS	CCS in both power and heat are all equipped after 2030		
Phase-out of fossil fuel in 2100 other than transport sector	0% in all the sectors in power, heat, hydrogen and fuel	No constraint	
Transport sector			
numbers of vehicles in 2100	70% EV, 30% FCV, 0% ICE and PHEV		
hydrogen in Aviation	50% and 100% in 2050 and 2100, respectively		
GMTR in 2100			
BAU	2.71DC (CO_2 only) 2.78DC (incl. GHG)	2.73DC (CO_2 only) 2.81DC (incl. GHG)	2.85DC (CO_2 only) 2.93DC (incl. GHG)
net ZERO	1.70DC (CO_2 only) 1.78DC (incl. GHG)	1.70DC (CO_2 only) 1.77DC (incl. GHG)	1.70DC (CO_2 only) 1.78DC (incl. GHG)

Note; each energy scenario accommodates both climate policies (i.e., BAU, net ZERO).

Table 2b
The three energy scenarios. (b) The Ren100 requires more stringent constraints in all the sectors and hydrogen use.

Settings and assumption \ Energy scenarios	Less constraints on all the sectors	100% CCS after 2030 in only power and phase-out in transport	CCS after 2030 in both CCS and transport	Ren 100
All equipped CCS in power	after 2050	After 2030		
All equipped CCS in heat	after 2050	No constraint	After 2030	
Transport sector (share of numbers of vehicles in 2100)	ICE; 1% PHEV; 14% EV; 65% FCV; 20%	ICE; 0% PHEV; 0% EV; 70% FCV; 30%	ICE; 1% PHEV; 14% EV; 65% FCV; 20%	ICE; 0% PHEV; 0% EV; 70% FCV; 30%
Hydrogen in Aviation in 2100	no constraint	100%	no constraint	100%
Hydrogen in Aviation in 2050	no constraint			50%
GMTR w.o/w NCGHG (net ZERO)	1.83/1.90 DC	1.84/1.92	1.78/1.86	1.70/1.78

pathways including Coal & Nuc (substantial increase in coal and nuclear).

The computation of changes in the energy scenarios was executed by simply changing data for gas and uranium resources and their production costs in obtaining Coal & Nuc and Gas & Ren, from which Ren 100 can be created by the additional constraints and phasing-out of fossil fuel. The two climate policy scenarios are (1) business as usual (BAU) with no emission control on greenhouse gases (GHGs), and (2) net ZERO emissions, whose cumulative emissions are zero over the time horizon using the cumulative emissions of Wigley Richels Edmonds (WRE) [43] 350 ppm constraints over the computational time horizon (from 2010 to 2150). The cumulative emissions constraints are capped in the net ZERO and restarted for computation from BAU solutions in each energy scenario.

Table 3
Data settings for metal requirement applied in this study.

Technology	Metal	Intensity of use of metals for installed capacity [t/GW]		Lifetime		Reference
		Maximum	Minimum	Default	Long	
c-Si PV	Si	6630	638	20	30	[97]
	Silver	36	19			[98]
CIGS PV	Indium	28	7			[97]
	Gallium	9	2			[97]
	Selenium	161	17			[97]
CdTe PV	Cadmium	138	17			[97]
	Tellurium	156	19			[97]
Wind	Copper	2000	1830	20	30	[47]
	Iron	140,000	135,000			[47]
	Neodymium	186	124			[46]
	Dysprosium	33	22			[46]
EV	Lithium	12.7 (kg/car)	2.4 (kg/car)	10	15	[45]
	Cobalt	8.8 (kg/car)	–			[45]
	Nickel	46.5 (kg/car)	–			[45]
	Manganese	91.5 (kg/car)	–			[45]
PHEV	Lithium	5.1 (kg/car)	1.4 (kg/car)	10	15	[45]
	Cobalt	3.5 (kg/car)	–			[45]
	Nickel	18.6 (kg/car)	–			[45]
	Manganese	36.6 (kg/car)	–			[45]
Nuclear	Hafnium	0.48	–	40	60	[99]
	Indium	1.6	–			[99]
	Silver	8.3	–			[99]
	Molybdenum	70.8	–			[99]
	Copper	2500	800			[100]
Geothermal	Copper	1300		50	60	[100]
	Copper	3050				[101]
Hydro	Copper	3160		30	40	[101]
Coal	Copper	890		30	40	[101]
Oil	Copper	1100		30	40	[101]
Gas	Copper	1110		30	40	[101]
Hydrogen	Copper	1110		30	40	[101]
Biomass	Copper	1210		30	40	[101]
CCS	Vanadium	100		30	40	[99]
	Niobium	100				[99]
	Nickel	1145				[99]
Trans.&Dist.	Copper	10,000		50	60	[100]
H_2 Production for FCV	Zirconium	325 (kg/t-H_2)	143 (kg/t-H_2)	30	40	[102]
	Palladium	2628 (kg/t-H_2)	88.6 (kg/t-H_2)			[103,104]
	Copper	825 (kg/t-H_2)	99.7 (kg/t-H_2)			[102]
	Silver	701 (kg/t-H_2)	26.3 (kg/t-H_2)			Coal or biomass-based membrane reactor [105]
	Aluminium	333 (kg/t-H_2)	115 (kg/t-H_2)			[102]
FCV cell	Nickel	2.4 (kg/car)	1.2 (kg/car)	10	15	[106]
	Zirconium	8.4 (kg/car)	1.2 (kg/car)			[107]
	Platinum	0.084 (kg/car)	0.024 (kg/car)			[108]
	Yttrium	2.4 (kg/car)	0.12 (kg/car)			[107]
FCV Tank	Nickel	132.0 (kg/car)	92.7 (kg/car)	10	15	[109]
	Zirconium	46.2 (kg/car)	42.5 (kg/car)			[110]
	Platinum	7.3 (kg/car)	0.066 (kg/car)			[111]
	Vanadium	57.4 (kg/car)	45.1 (kg/car)			[110,112]
	Titanium	37.7 (kg/car)	5.2 (kg/car)			[109]
	Aluminium	281.2 (kg/car)	14.1 (kg/car)			[109]
	Lithium	0.87 (kg/car)	0.54 (kg/car)			[111]
	Lanthanum	62.4 (kg/car)	49 (kg/car)			[109]
	Magnesium	98.8 (kg/car)	38.8 (kg/car)			[109]
	Copper	0.017 (kg/car)	0.017 (kg/car)			[109]
	Chromium	0.024 (kg/car)	0.024 (kg/car)			[111]
	Boron	11.8 (kg/car)	11.7 (kg/car)			[111]
	Tungsten	0.031 (kg/car)	0.031 (kg/car)			[111]

Note: Capacity factors are given as follows; 85% for power generation by fossil fuels, hydrogen, biomass; 75% for nuclear; 70% for Geothermal; 50% for wind; 45% for hydro; and from 17% in 2010 to 40% after 2050 for PV.

3.3. Assumptions of metal requirements and availability

Table 3 summarizes data sets – (i) intensity of use (IU) of metals and (ii) lifetime (or service years) - for various technologies including hydrogen related technology. In addition to these, the following factors are generally subjected to uncertainty in the estimate of metal requirement and availability: (iii) the rate of reduction or improvement of IU of metals, (iv) end-of-life (EoL) recycling rate, and (v) share of the technologies in the same category. Critical appraisal or further reviews of these data was out of the scope of this study.

We estimated both maximum and uncertainty ranges for the metal requirement and availability. In the maximum estimate, the maximum IU of metal and no reduction rate (meaning no progress in reducing the amount of metals used per unit output) is assumed. The uncertainty ranges between levels in the maximum and minimum are calculated by the following settings in Table 3: (i) minimum level of IU among various estimates, (ii) longer lifetime of the technology and (iii) reduction rate in IU and improvement rate in EoL recycling rate, both set as 1%

per annum. Levels were determined by a review of relevant literature for (i) and (ii) while assumptions were made for (iii) based on our background information.

The share of technology in PV (above mentioned as v)) is taken into consideration as the following two compositions: one with 100% crystalline silicon (c-Si), the other with 50/50% of copper-indium-gallium-selenium (CIGS) and cadmium-tellurium (CdTe) over the time period. The metal requirement is calculated by multiplying additional (newly-built) capacity of energy technologies with the intensity of use of metals in the technologies. In the calculation of cumulative production, the lifetime of the additional capacity and recycling rate is accounted for as a reduction in the amount of mined resources due to increase in the EoL recycling rate.

4. Results

4.1. Scenarios on power mix structure for the energy and climate policies

We start from Fig. 3 illustrating the power mix structure for produced electricity (in exajoules (EJ), where 1 EJ = 10^{18} J), for the six combinations of energy and climate policy. Here we focus on the Ren 100 while the other two, discussed detailed in our former publication [1], are shown for comparison. In order to find computational solutions (optimal - economically efficient) for all combinations of the policies, the operation windows are made as wide as possible. Through our modeling exercise to obtain feasible computational solutions to meet the well-below 2 °C target, all the parameter settings are common in the three scenarios, except that by changing the data for resource supply cost (i.e., uranium, gas) in Ren 100 allowing further expansion of renewable energy while simultaneously phasing out nuclear and fossil fuels in the power and heat sectors.

Ren 100 can be characterized through the following issues. Further expansion of renewable energy technologies, almost doubling from Gas & Ren in Ocean, Wind (offshore), PV, biomass, and geothermal. This is almost tripled when compared with Coal & Nuc where Ocean and Wind (offshore) is introduced. Another feature is less dependency on CCS in Ren 100, unlike the other two under the net ZERO scenarios where all the fossil fired power plants are equipped with CCS. Net ZERO shifts the power mixture by reducing coal (in Ren 100), CCS equipped fossil fired (in Gas & Ren, Coal & Nuc), and expanding nuclear (in Coal & Nuc), respectively. We recognized in Ren 100 that in order to attain the net ZERO climate policy scenario, a tremendous increase of renewable energies are required, while phasing out of fossil powers when compared with BAU.

Fig. 4 illustrates additional (new) capacity of the power mix in Tera Watt per year (TW/yr), which is converted from Fig. 3 by dividing each plant capacity factor by 8760 h annually. The capacity increase in Ren 100 is apparently higher compared with those in the other two (1.9 versus 1.2 TW/yr, around 50% greater) which is due to large-scale deployment of PV and WP (8–9 and 3 times in Ren 100 higher than the other two) with lower capacity factors in order to meet the power demand, which is identical among the three.

Fig. 5 illustrates the global CO_2-equivalent (CO_2eq) balance and global mean temperature rise (GMTR) under the three scenarios, by using lines (red for CO_2eq emission, blue for GMTR) and by bar graphs only for Ren 100 (positive for emissions, negative for deployment of CCS in various sectors). The upper red lines (emissions) of BAU in Ren 100 (two dots, dashed) shows a similar trajectory up to 2050 with Coal & Nuc (dashed with one dot), but thereafter dramatically drops due to the great expansion of the renewables. Because of this radical emissions reduction, the amount of CCS peaks after 2050. Although the three pathways in BAU (red lines) differ greatly, surprisingly the GMTR in BAU are almost identical at the end of 2100, implying three “extreme” energy directions will lead us to similar degrees of “warming” world. The lower red lines (almost identical) indicate peaking of emissions within a few decades.

4.2. Metal requirement and availability

4.2.1. Presentation of results

Results of metal requirement and availability are presented as follows in this section. Annual metal requirement in 2100 is compared with resource production in 2015. This is commonly presented in the left side of the figures in this section, while on the right side cumulative production over the time horizon is compared with resources of the metal. For each metal, three bars are presented, corresponding to “Coal &Nuc”, “Gas&Ren”, and “Ren100”, from left to right respectively. The upper part of each bar, where color and texture are differentiated from the remaining, corresponds to the uncertainty ranges, identical to the amount of metals reduced by the settings described previously. The ceiling of the sum of all the bars corresponds to the maximum amount of each metal requirement.

Most data compared with the estimations from our model are sourced from USGS reports [44]. However, the metal requirement for some elements (Nd, Dy, La, and Ce) are projections from a DOE report [45] from those in 2010 level and others [46], while for availability of some elements (In, Ga, Cd) data is obtained from [47,48]. The results are presented, first by technology type (renewable energy and hydrogen related) for the requirement and availability; then commonly used metals of the technology types (i.e., silver, indium).

4.2.2. Technology type

Fig. 6 displays various metals required for PV. Consistent with the large-scale deployment of PV, requirement of all metals in Ren 100 (top right in each set of three bars) are the highest among the three. In the metal requirement in 2100, some metals (Silicon, Silver, Cadmium, Copper) are close to, reaching, or above the total production in 2015, respectively, excluding the uncertainty (i.e., maximum level). Simultaneously, uncertainty ranges indicate potential large reductions in the metal requirement and thus the cumulative metal production; in some metals the ceiling is lowered by the uncertainties to far lower than the 2015 production as well as below the level of resources (e.g., Silver, Selenium, Cadmium, Gallium).

Fig. 7 indicates metal requirement and availability for wind power (WP). The metal requirement and cumulative production do not differ among the three scenarios as widely as compared with PV in Fig. 6. Neodymium and Dysprosium show lower amounts of 2100 metal requirement than 2015 production. However, metal requirement and availability in other metals are far below the levels of their 2015 production and resources.

Fig. 8 provides results for FCV. The metals required for fuel cells are only Nickel, Zirconium, Platinum, and Yttrium (the most left), while other metals are for H_2 production and tank for FCV. This result remains unchanged when commonly used metals for hydrogen stations are included (Zirconium, Copper, and Aluminum). The metal requirement and availability among the three scenarios are identical. More than half the metals exceed either metal requirement in 2100 (compared with 2015 production) or cumulative production (with resources) *without* the uncertainty ranges, while Nickel, Zirconium, Lanthanum exceed when uncertainties are taken into consideration. Specifically for Platinum and Vanadium, both levels of the 2015 production and the resources are well below the uncertainty ranges, implying that these are candidate potentially critical metals.

4.2.3. Commonly used metals and resources

Fig. 9 illustrates results in commonly used metals in Nuclear, PV, CCS, (PH)EV, and FCV, across the three energy scenarios. These include Silver, Indium, Vanadium, Niobium, Nickel, and Lithium; while Copper is excluded since our previous investigation [1] clarified that Copper metal requirement is well below levels of 2015 production and resources.

Vanadium (used in CCS, (PH)EV, FCV) is identified as *distinctly* critical in the sense that the production level in 2100 and cumulative

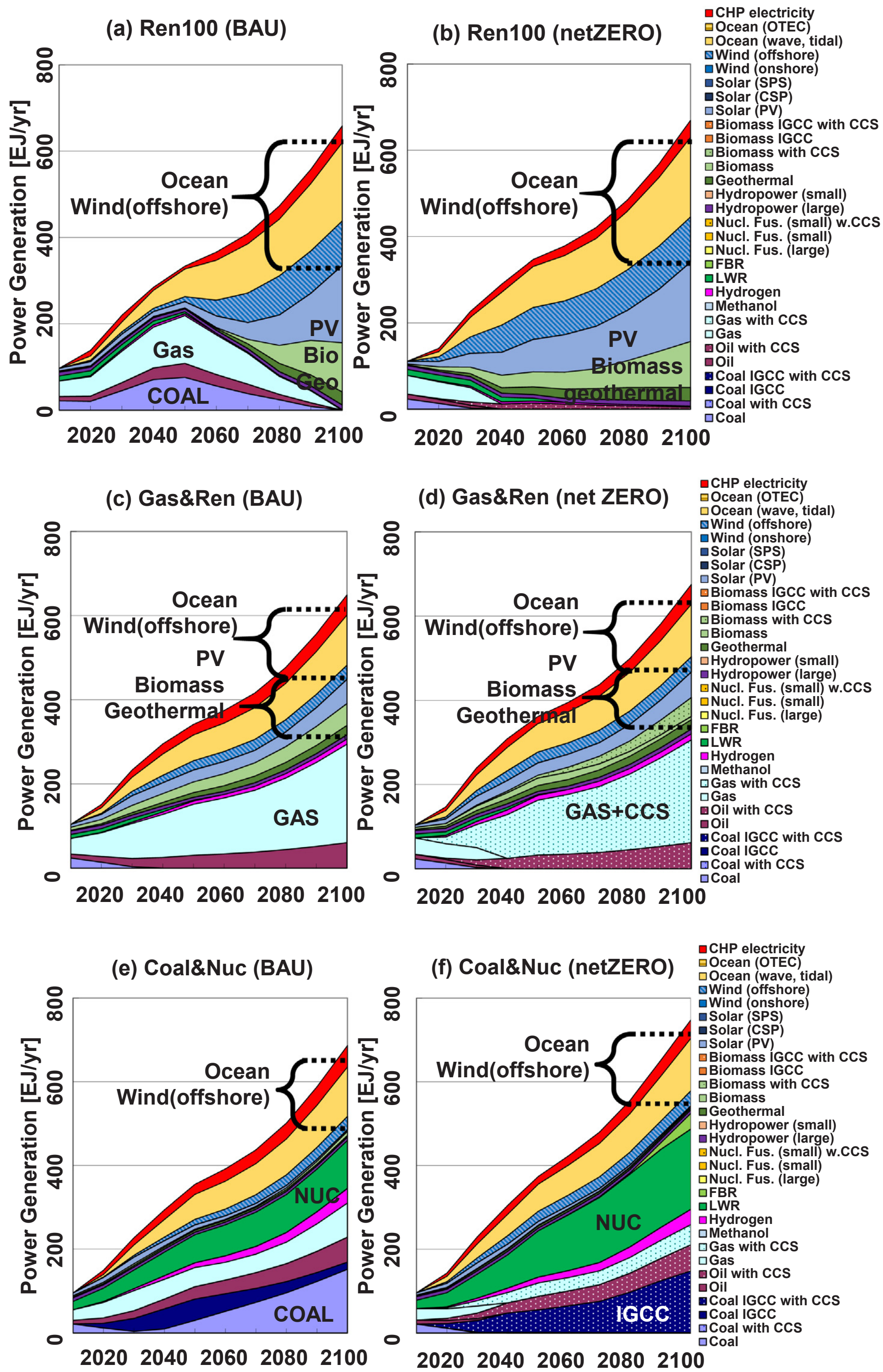

Fig. 3. Global power supply structure under the three energy scenarios with two climate policies.

production well exceed the levels of production in 2015 and resources respectively, across all the three scenarios. Indium (in (PH)EV, FCV) and Nickel (in CCS, (PH)EV, FCV)) are the next candidates in the cumulative production. Lithium (in (PH)EV, FCV) for those levels is within the uncertainties across the three energy scenarios, succeeded by Silver and while Niobium is uncritical.

4.3. Fossil fuel availability

Estimates of fossil fuel resources used in this study are based on the compilations and reviews undertaken by McGlade [49] and McGlade and Ekins [50], supplemented with updated figures from IEA (International Energy Agency) [51] and BGR (Federal Institute for Geosciences and Natural Resources) [52], Rogner et al. [53], and Rogner [54]. Data presented in IPCC-AR5 and Global Energy Assessment are sourced from Rogner et al. [53] while our given data is compiled from Rogner [54], from which numbers in gas are multiplied by fivefold only in the Gas&Ren scenario for implying “cheap gas”.

We use the same definition of ‘resources’ as [50]. That is, ‘resources’ are used as shorthand for remaining ultimately recoverable resources

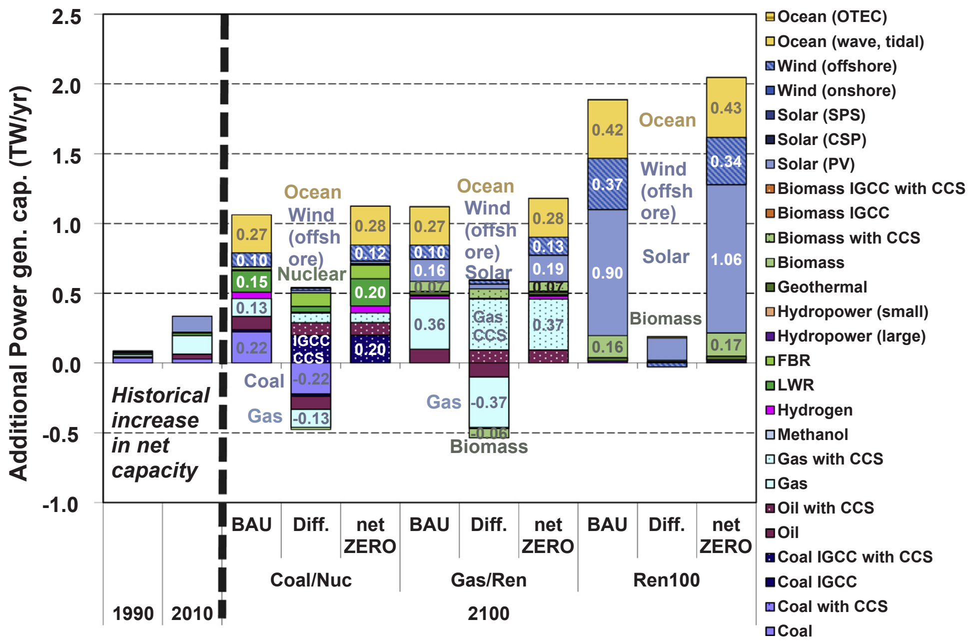

Fig. 4. Additional capacity increase in BAU and net ZERO, and difference between them (Diff.) in 2100, and historical increase (1990, 2010) in net capacity under the three energy scenarios.

(RURR). Estimates of RURR are estimates of remaining amounts of oil, gas and coal believed to be recoverable over all time, including with future technology and under future economic conditions. 'Reserves' are a subset of resources that is estimated to be recoverable with today's technology and market conditions. Since our study is long range (the model runs up until 2150) resource estimates are of main interest. Hence, reserves estimate are only studied as part of the total resource estimate.

The McGlade-reviews include high, median and low resource estimates for different categories of oil and gas, and a central estimate for coal resources. Table 4 presents aggregated resource estimate from McGlade, IEA, BGR, and Rogner, comparing our given data and results by model runs. McGlade RURR estimate are as of 2010, while IEA and BGR are of 2016, for exact comparison (out of scope in this study) these figures have to be adjusted by historical cumulative production during the intervening years. Our given data to the model and computational results under the three energy scenarios are confirmed to be within the ranges of various resources estimates, implying that energy scarcity is less likely compared with minerals assessed in this study.

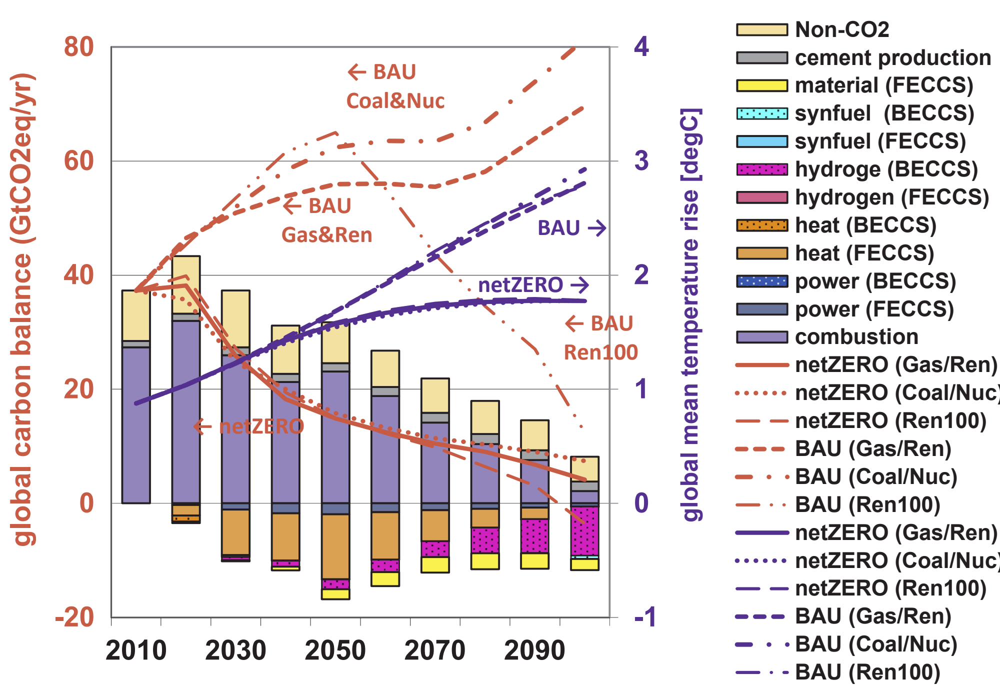

Fig. 5. global carbon balance and global mean temperature rise.

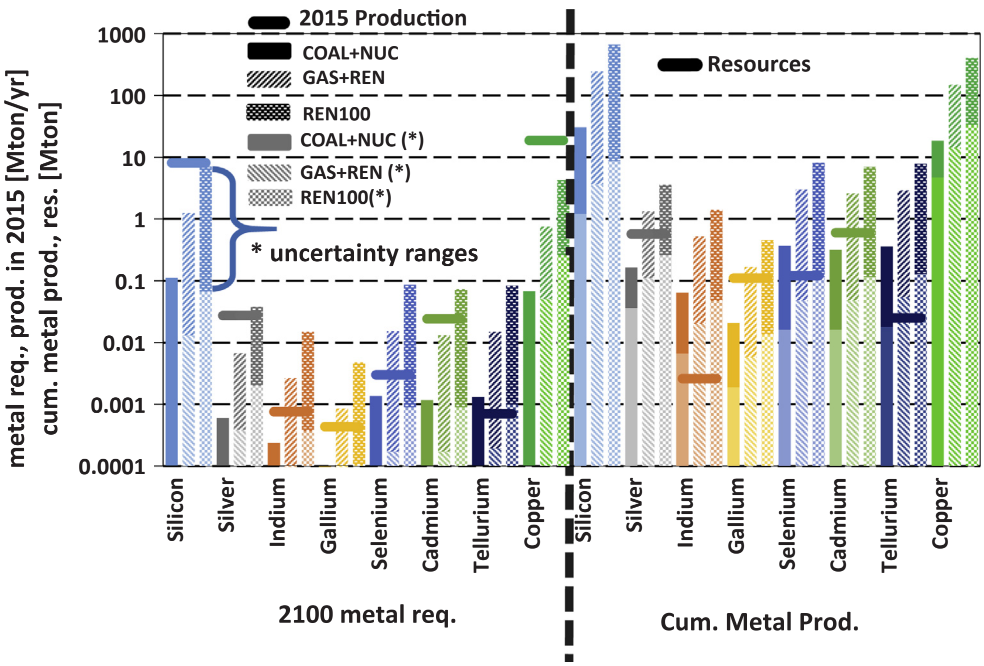

Fig. 6. PV; Annual metal requirement, metal production in 2015, cumulative production, resources.

5. Discussions

5.1. The Ren 100 scenario

Although our setting for Ren 100 drastically expanded the allowable maximum capacity for renewables, the decarbonization in total primary energy supply (TPES) arrives at 2100, not 2050. This means that the maximum capacity of renewables expand its capacity only in the latter half of this century because of relatively expensive cost of renewables, implying that enforcement in further deployment of renewables may be required. Such a 100% renewable scenario shares the common issue of variable renewable energy (VRE) in power systems. Our Ren 100 scenario can also be characterized as lower dependency on CCS compared with Gas & Ren (less than 20 Gton of CO_2 per year in Ren 100 while exceeding 40 in Gas & Ren). This implies that unsuccessful deployment of large scale CCS in coming decades requires radical expansion of renewables demonstrated in this study. Some other comments on this energy scenario are also given here. We assumed that the Ren 100 scenario is not compatible with the use of nuclear power, hence nuclear phase-out is also added.

Our Ren 100 scenario can also be compared with other existing studies. The WWF energy scenario [55] assumed the baseline total final energy demand gradual increase to 520 EJ/yr in 2050 while ours is a little higher, at some 670 EJ/yr. It is, however, the WWF scenario gave

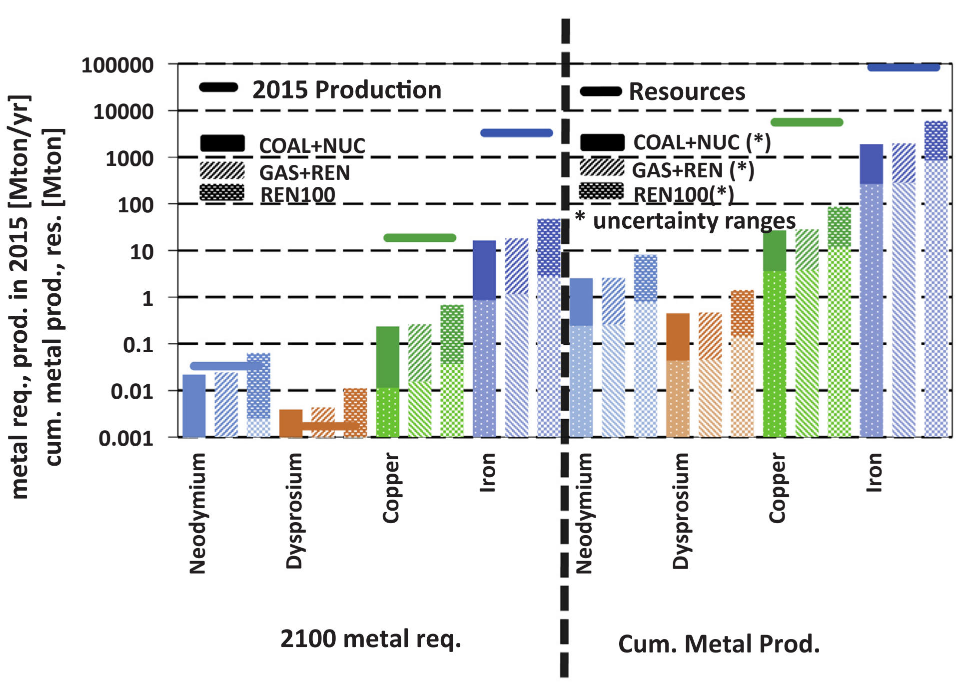

Fig. 7. WP; Annual metal requirement, metal production in 2015, cumulative production, resources.

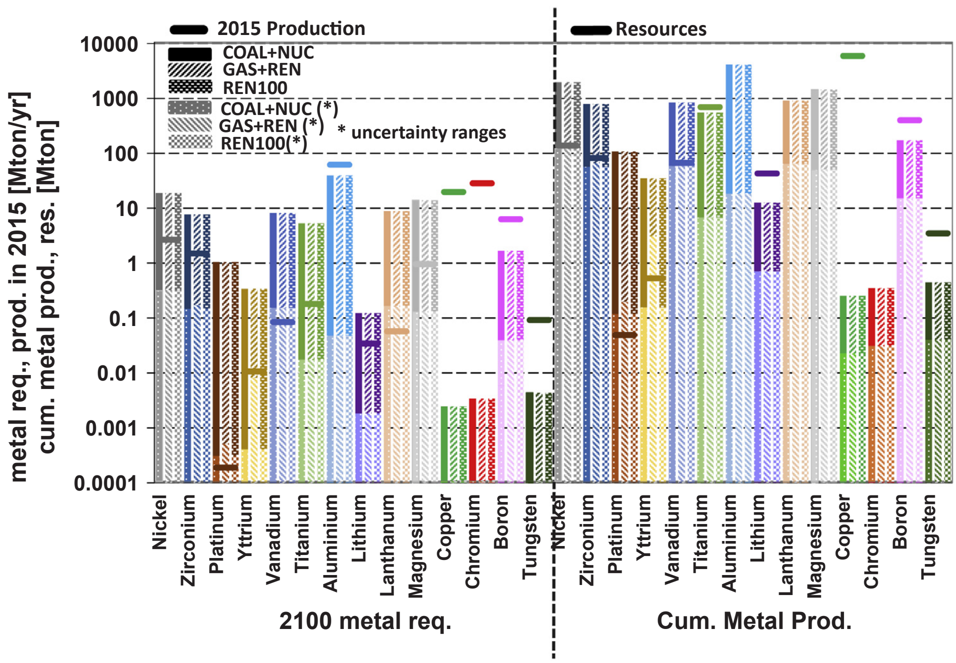

Fig. 8. FCV; Annual metal requirement, metal production in 2015, cumulative production, resources.

aggressive energy conservation allowing its peak out at 350 EJ/yr in 2020 to stabilize at 260 EJ/yr (of which 250 by renewables while ours is some 240), identical to its level in 2000. Our result in 2050 by Ren 100 can be summarized that dependency on renewables is comparable to the WWF energy scenario while other energy sources are added onto that to meet the total energy demand. The International Renewable Energy Agency (IRENA) REmap 2016 scenario [56] illustrates a target share of renewable energy share in total final energy consumption in 2030 of 36% in their REmap case (116 EJ/yr in total) while ours is some 34% (some 500 EJ/yr for electricity, heat, and transport). The scenarios indicates that in 2050 TPES ranges between 475 and 700 EJ/yr, of which 52–60% is shared by renewables (ranges 195–240 EJ/yr) while ours is 1100 EJ/yr with 45% share by renewables (240 EJ/yr). The 45% share is lower than Greenpeace's energy revolution (over 70%) [57] and scenarios in Global Energy Assessment (GEA) [58] (close to 50–60%) while larger than those by Shell [59] and World Energy Council (WEC) [60].

5.2. Metal requirement and availability

Our exercises clarify significant metal requirements in PV in Ren 100 and (*ad-hoc*) uncertainty ranges in various metals and technologies. As indicated by Fig. 4, PV is the largest difference among the three scenarios and Ren 100 shows the largest for the additional capacity

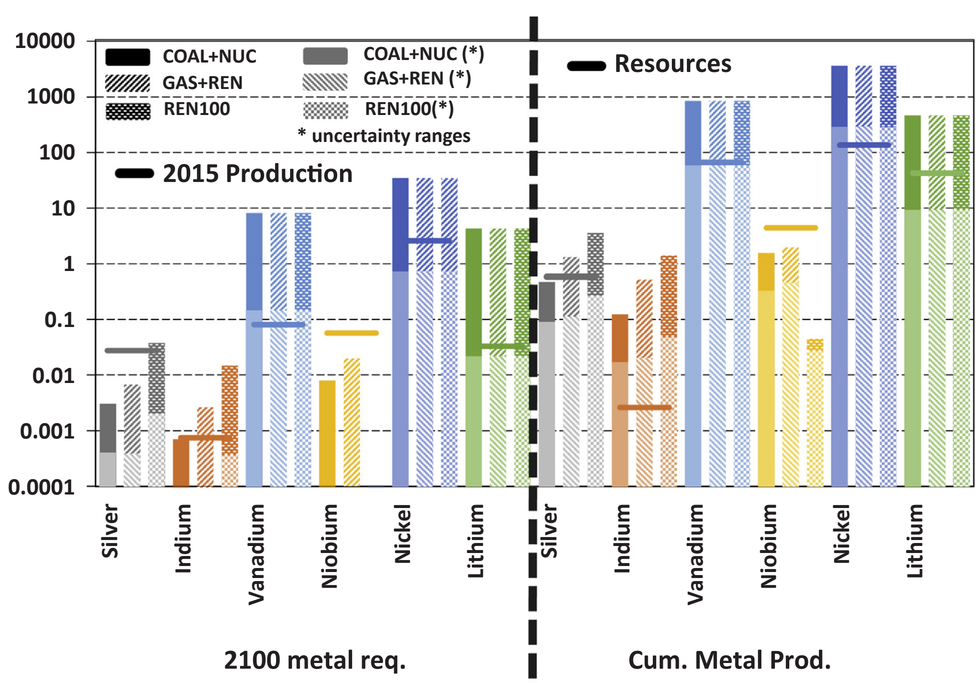

Fig. 9. Silver, Indium, Vanadium, Niobium, Nickel, Lithium; Annual metal requirement, metal production in 2015, cumulative production, resources.

Table 4
Assessment of fossil fuel resources; various sources and our study.

Reserves + Resources	Various sources and ours																
	McGlade and Ekins [50]			IEA [51]	BGR [52]	Rogner et al. [53]			Rogner [54]	Data given in this study		Cumulative production in this study					
												BAU			net ZERO		
	Low	Median	High	Central	Central	Min	Median	Max	Resource base	Resource	Resource × 5	Ren100	Gas/Ren	Coal/Nuc	Ren100	Gas/Ren	Coal/Nuc
Oil conventional	9253	13,223	18,221	15,782	14,234	9070	11,415	13,760	12,351	10,647		7590	7590	7590	7590	7590	7590
Oil unconventional	8168	15,737	25,476	19,329	14,046	15,030	17,715	20,400	21,729	24,585		3936	5149	6572	1607	4002	4990
Total oil	17,422	28,960	43,697	35,112	28,280	24,100	29,130	34,160	34,081	35,232		11,527	12,740	14,162	9197	11,592	12,580
Gas conventional	10,175	13,875	17,945	15,984	11,951	12,200	14,100	16,000	17,585	10,730	53,648	20,052	30,417	9175	12,367	34,573	9175
Gas unconventional	7400	11,100	15,355	13,505	19,869	60,300	124,650	189,000	18,841	16,162	80,812	0	3080	7336	3	5069	6404
Total gas	17,575	24,975	33,300	29,489	31,820	72,500	138,750	205,000	36,425	26,892	134,459	20,052	33,497	16,511	12,370	39,641	15,579
Hard coal		75,174		535,186	438,705												
Lignite		17,151		53,088	20,028												
Total coal		92,325		588,274	458,733	308,300	382,150	456,000	142,351	95,920		10,587	13,934	27,313	3870	5184	21,258

Note; all the numbers in EJ unit. The following aggregates include: Oil conventional = current conventional 2P reserves, reserve growth, undiscovered oil, Arctic oil, natural gas liquids. Oil unconventional = tight oil, natural bitumen, extra-heavy oil and kerogen oil. Gas conventional = current conventional 2P reserves, reserve growth, undiscovered gas, Arctic gas. Unconventional gas = tight gas, coal-bed methane, shale gas. For Rogner et al. [53] and Rogner [54], use similar but not identical aggregates, most importantly if tight oil is included in conventional or unconventional. See references for exact definitions.

among them while no addition of PV in Coal & Nuc. The metals in PV by Ren 100 further requires by more than several compared with Gas & Ren, approaching or exceeding levels in the 2015 productions (silicon, silver, cadmium) while below in Gas & Ren. Except for bulk metals (silicon, copper), all scarce metals in PV exceed the level of resources in both energy scenarios (Ren 100, Gas & Ren). However, in Coal & Nuc, cumulative production levels in only Silver, Gallium, Cadmium are well below their resources levels.

Unlike PV, constraints from metal requirements and availability in WP seem lower, since only Dysprosium requirement in 2100 is far beyond 2015 production level and Neodymium in Ren 100 slightly exceeds the level. This observation implies that the technology choice of PV is less while WP is more compared with those illustrated in Ren 100.

The more than half of the metals in FCV, and all the metals in (PH) EV, are well exceeding both the 2015 production in 2100 metal requirements and resources in cumulative metal production. The share in the Table 1 (30 and 70% each) corresponds to 1.2 and 3 Billion of vehicles for FCV and (PH)EV respectively in 2100. Some metals do not exceed their 2100 metal requirement (e.g., Lithium in FCV, Manganese in (PH)EV), when (dramatically but potentially unrealistically) assuming the number of the vehicles reduced by one-tenth, but still some well exceed their the 2015 production level (e.g., Platinum in FCV, Lithium in (PH)EV). In this sense, both FCV and (PH)EV will be faced with limitations of availability when they are largely shared in a market under the assumption of maximum metal requirement.

We stress that the results discussed above suggest a variety of implications for metal use in the technologies (i.e., metal use saving) and technology choices for climate change mitigation in covering any energy direction under the three extreme energy scenarios.

6. Conclusions

We summarize our modeling exercise to meet the well-below 2 °C target and its metal requirement in this section.

- [meeting the well-below 2 °C target] Including or excluding non CO2 Greenhouse gases is the key to attain the 2 °C target and energy mix strategy. Although the contrasting three energy policies - namely 100% renewable energy (Ren 100), Gas & Ren, Coal & Nuc - well below 2 °C when *excluding* and including non CO2 Greenhouse gases by the power sector solely even under the net ZERO climate policy. This implies that across the three energy scenarios our model requires, in addition to the power and heat sectors, the transport sector to be fully decarbonized, comprising of Electric Vehicles, Fuel Cell Vehicles, and hydrogen aviation to meet the well-below 2 °C target including non CO2 Greenhouse gases.
- [Technology choice] Technology choice in Ren 100 shows contrasting characters as follows when compared with the other two energy policies. Photovoltaics cause the largest difference by orders of magnitude, followed by Wind Power and ocean power by a few factors, and minor difference in the transport sector. Cumulative amount of CO2 storage is the lowest by one fourth thanks to the dramatically expansion of the renewable technologies.
- [Metal requirement] The following mineral elements may be candidates to be classed as "critical" among the three energy policies with uncertainties; namely Selenium, Indium, and Tellurium in Photovoltaic; Dysprosium in Wind Power; Nickel, Zirconium, Platinum, Yttrium, Vanadium, Lithium, and Lanthanum in Fuel Cell Vehicle. Underlined elements are relatively critical in the sense that cumulative metal production well-exceeds the resources level in all the three scenarios and the uncertainties. This may suggests that less scarce metal intensive technologies such as Wind Power and (Plug in Hybrid) Electric Vehicle are better for consideration than relatively more metal intensive ones. Silver, Indium, Vanadium, Niobium, Nickel, and Lithium are commonly used metals in Nuclear, Photovoltaic, Carbon Capture and Storage, (Plug in Hybrid) Electric

Vehicle, and Fuel Cell Vehicle. Vanadium is identified *distinctly* critical in the sense that production level in 2100 and cumulative production well exceed the levels of production in 2015 and resources respectively across all the three scenarios and the uncertainties. Indium and Nickel are the next candidates for scarcity, followed by Lithium.

Our modeling exercise suggests that (i) carbonization by all the sectors are essential to achieve well-below 2 °C target under the representative three energy policy scenarios, (ii) Vanadium is *distinctly* “critical” across the three energy policies commonly used in the technologies (Nuclear, Photovoltaic, Carbon Capture and Storage, (Plug in Hybrid) Electric Vehicle, and Fuel Cell Vehicle), and (iii) Tellurium, Zirconium, Platinum, and Indium are “critical” for respective technologies.

We stress our originalities in this studies are those findings, employing an energy model for the energy-mineral nexus study, and scenario building flexibility in energy and climate without borrowing from authorities (e.g., Ren 100, net ZERO). The collaboration of both communities in the energy-mineral nexus bring great benefit to policy makers and research scientists for better understanding and decision making in policy. The uncertainties for the metal requirement are taken into consideration while climate related (e.g., with/without non CO2 Greenhouse gases, carbon accounting, climate sensitivity) remain as future tasks.

Acknowledgements

The first author gives his deepest thank to National Institute of Advanced Industrial Science and Technology (AIST) and Arai Science and Technology Foundation for supporting this work. MH and HW have been supported by the Swedish Research Council (project number 2014-5246) and by the Swedish strategic research program StandUp for Energy.

Appendix A. Review of established hydrogen production techniques

A.1. Hydrocarbon reforming

Catalytic reforming or gasification of fossil fuels are the most common process routes to obtain hydrogen but roughly 7 kg of CO_2 per kg of H_2 are produced and emitted into the atmosphere [61]. The widespread use of steam-methane reforming (SMR) relies on natural gas as a feedstock. Other catalytic approaches such as autothermal reforming (ATR) and partial oxidation (POX) are also mature and proven commercial technologies with significant shares of world hydrogen production. POX can be used with lower quality feedstocks such as coal, petroleum coke and other residues from fossil fuel processing. Energy efficiencies of SMR, ATR and, POX can be in the range of 60–84% [16,62–65]. These efficiencies would be lowered if carbon capture and storage were to be implemented, just as in the case of power plants [66]. SMR, ATR, and POX all require substantial energy inputs and generate significant carbon dioxide emissions, due to the high endothermicity of fossil fuel-based reforming and gasification processes.

Some emerging hydrogen production methods are available and have entered early phases of commercialization. These include non-oxidative processing of hydrocarbons that strives to avoid COx formation by having no oxidants such as H_2O or O_2 in the system. The achievement of this typically requires very high temperatures and a catalyst. One such approach is thermal plasma systems, which employ high temperature plasma (5000–10,000 °C) to perform methane decomposition into hydrogen and carbon, an approach which was commercialized in 1999 by the Norwegian company Kværner in its Carbon Black and Hydrogen (CB&H) process. Industrial plasma reformers with a high degree of heat regeneration could be expected to consume around ∼15–20 MJ/kg H_2, while typical lifetime depends on electrode erosion caused on the coaxial graphite electrodes used in the Kværner process. Reported erosion is in the order of 0.1 g/kWh [67]. If the produced carbon black is sufficiently pure to be useful for toners, tires and paint industry, the CB&H process can be commercially competitive with SMR despite higher energy consumption. Plasma reforming is covered in reviews by Chen et al. [68] and Lee [69]. Plasma reforming could be expected to become more widely used in the future due to its compactness, environmental characteristics, and ability to use difficult fuels such as raw biofuels or heavy oils [70].

Non-fossil thermal approaches to reforming hydrocarbons also exist. Gas-cooled reactors capable of delivering high temperature process heat (750–1000 °C) together with SMR and Pd-based membranes were found to increase final product yield compared to conventional SMR plants [71]. Nuclear heat for methane decomposition using molten metal baths could be a cost-effective option for Generation IV reactor designs [72]. Solar thermal systems with SMR and Ni/Al_2O_3-catalysts were found to reach promising results at temperatures less than 1000 °C [73,74]. However, such approaches do not yield any noteworthy commercial output at present and will likely require long lead times before they can produce any major share of world hydrogen supply (see Fig. A1).

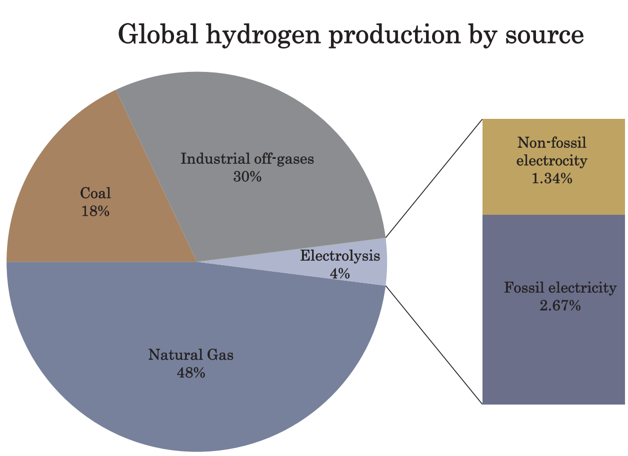

Fig. A1. Global hydrogen production by source. Data taken from IEA [75] and electricity is divided into fossil and non-fossil parts using IEA [51].

Table A1
Typical flow rates, and composition of steelwork off-gases after cleaning in a modern steel plant producing 6 Mt steel/year. Adapted from: Uribe-Soto et al. [78].

	Coke-oven gas	Blast furnace gas	Basic oxygen furnace	Mix
Volumetric flow rate [m_3/h]	40,000	730,000	35,000	805,000
Thermal power [MW]	174	682	70	926
Compound	Basis molar fraction (%)			
CO_2	1.2	21.6	20.0	20.5
CO	4.1	23.5	54.0	23.9
H_2	60.7	3.7	3.2	6.5
CH_4	22.0	0.0	0.0	1.1
C_xH_y	2.0	0.0	0.0	0.1
N_2	5.8	46.6	18.1	43.3
H_2O	4.0	4.0	4.0	4.0
Ar + O_2	0.2	0.6	0.7	0.6

A.2. Industrial off-gas streams

Industrial off-gas streams also account for a major share of world hydrogen output, and tend to be heavily reliant on fossil fuels. Today, hydrogen is currently used in industries spanning from chemicals and refining to metallurgy, glass, and electronics. Most off-gases that are used for hydrogen recovery are derived from petrochemical plants, ethylene crackers, and metal processing [75]. However, most of the industry generated hydrogen is also consumed onsite and never enters any commercial hydrogen market [14].

Hydrogen has increasingly been used worldwide to upgrade heavy oils, generate more valuable refined products and to remove sulphur and nitrogen from fuels to meet stricter quality/environmental requirements [13]. This consumes large volumes of hydrogen and many refineries and petrochemical plants already face rising demand and shortfalls of hydrogen. Typically, the cost of hydrogen for these operations is only surpassed by crude oil [76]. It appears unreasonable that any net surplus of hydrogen could be obtained from petrochemical off-gas streams, even though more efficient processes management could alleviate some H_2 demand.

Another potential off-gas stream could arise from the steel industry. A total of 74.3% of all world steel production relies on the integrated route using both blast and basic oxygen furnaces [77]. This generates streams of off-gases with significant concentrations of reducing agents such as CO, CH_4 and H_2 that can be recovered (Appendix Table A1). Coke-oven gas may have high concentrations, but smaller volumes compared to blast furnace gas. Steelwork off-gases also contain undesirable compounds such as dust, aromatics and H_2S or HCN. Additional gas treatment stages are often necessary for potential exploitation of such off-gases, since most of these compounds are catalyst poisons. Coke-oven gas is in many cases the only available off-gas, due to favourable economics and practicality [78]. It should be noted that in many countries there are already moves to utilize such off-gases, but mainly through direct combustion for energy recovery.

Another mature industrial off-gas stream is from the chlor-alkali industry that produces chlorine, sodium/potassium hydroxide, and hydrogen via electrolysis of brine. This process is highly energy intensive, which is a key concern for this industrial sector [79]. A new direction for reducing electrolytic energy use is replacing the traditional hydrogen evolution cathode with an oxygen depolarised cathode (ODC). Although this shift increases energy efficiency up to 30%, it requires pure oxygen as a raw material and does not co-produce hydrogen [80]. There is a risk that hydrogen streams from this off-gas sector will dry-up in the future if more ODC-technology is pursued by the chlor-alkali producers.

Some new industrial off-gas streams are for example in solar cell production. Chemical vapour deposition (CVD) is one of the current methods for producing solar cells where silicon semiconducting layers are typically produced by using gaseous silicon compounds such as silane (SiH_4) and chlorinated silanes [81]. The hydrogen concentration in the off-gas stream from this process is ≥95% and potentially exploitable for hydrogen recovery using novel approaches [82]. If PV expands rapidly in the future, these off-gas streams may increase in importance for hydrogen production.

A.3. Electrolysis

Only a minute proportion of all H_2 is directly produced via electrolysis of water, which can be far more environmentally sensible if the electricity is obtained from renewable sources. At one time, it was actually the dominant hydrogen producer before low gas prices and SMR outperformed it in decades when carbon emissions were disregarded. Renewable hydrogen may be obtained from water electrolysis using energy gained from energy sources such as wind, solar or biomass, but high energy requirements (5.6 kWh/m^3H_2) are prohibitive and typical electrolyser energy efficiencies are only 56–73% [83]. The amount of electrical energy required can be reduced by the utilization of heat (preferably waste or renewable heat), thus improving the value proposition of hydrogen.

A.4. Other methods

Thermochemical splitting of water occurs at high temperatures via a series of chemical reactions and could be one method to reduce the reliance on hydrocarbons [84]. Suitable cycles such as sulphur-iodine or bromine-calcium can lower required process temperature to below 1000 °C [85], but very few have evolved beyond theoretical calculations to working experimental demonstrations that establish scientific and practical feasibility of the thermochemical H_2 production [86]. More specifically, a Sandia report found that nearly all cycles under development have single-point failure challenges whose successful prosecution would be necessary for the cycle to promise competitive performance [87]. Such technologies are not likely to be commercialized and deployed on large scales for several decades into the future [75].

Different biological systems are also possible as genetic engineering and tailoring of microorganisms could allow feasible hydrogen production from organic matter [88]. However, much research is still needed to improve yields and make it more productive as this approach is far from commercially feasible within the foreseeable future [75].

A.5. Future trends in industrial hydrogen production

It has been the aim of researchers and policy-makers to encourage the production of hydrogen from renewable energy, the fact remains that the majority of hydrogen today is produced from either natural gas (NG), coal or oil, and that most hydrogen is not used for either generating power or as a transportation fuel, but for hydrocracking of oil or for the production of ammonia. A number of key reasons are behind this lag in development, chiefly, the production of hydrogen from renewables has remained too inefficient and costly, the storage of hydrogen for onboard use in vehicles has not met the requirements of gravimetric and volumetric storage density to enable sufficient vehicle range [89], and the utilization technology, principally fuel cell technologies, have not reached sufficient commercial scales of production or competitive costs [90].

Hydrogen is still attractive because it shares a number of potential distinctions that separate it from competing technologies, despite this lag. Notably, the utilization of hydrogen in vehicles particularly offers a non-carbon, low-polluting technology that is likely to outcompete batteries in longer range transport [91], and hydrogen also offers a useful storage media for longer-term storage of energy, with potential advantages for inter-seasonal storage of excess electricity at a large scale, in comparison to batteries that provide excellent short-term storage.

One of the key barriers for hydrogen is the round-trip efficiency of electrolysis, storage and utilization – for example, standard alkaline electrolysis has an efficiency of around 80%, storage requires different energy inputs depending on the type of hydrogen storage, then the re-conversion of hydrogen to electricity through a high efficiency fuel cell is around 60% efficient at best – even neglecting the storage, this is an efficiency of less than 50%. Compare this to pumped hydro (70–80% for the pumping then ~95% for generation giving around 70–80% round-trip [92] or batteries (potentially up to 90% for Li-ion chemistries [93] or around 70–80% for lead acid batteries [94]. So while hydrogen may be useful for long-term storage, there are other technologies that will be more efficient in many cases. Concurrently, the rapid reduction in the cost of batteries (particularly lithium ion chemistries that still retain the best performance on efficiency, lifetime and weight) is seeing some of this competitive edge reduced, although there is still considered to be potential for hydrogen in certain markets [95], and its versatility for use in thermal, electric and chemical applications maintains interest [96].

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